

JS 9/15/21
RJA 01/18/22

SAT Report for Case # P-18-0152

General

Report Status:	Complete	Status Date:	11/27/2018
CRSS Date:	04/30/2018	SAT Date:	05/02/2018
Consolidated PMN?	N	SAT Chair:	William Irwin
Consolidated Set:			
Submitter:			
CAS Number:			
Ecotox Related Cases:			
Health Related Cases:			
Chemical Name:			
Use:			
Trade name:			
PV			
Max (kg/yr):			
Ecotox Assessor:	Nguyen, Amelia	Fate Assessor:	Lee, WenHsiung
		Health Assessor:	Jacobs, Keith

Physical Chemical Information

Molecular Weight:		Physical State - Neat:	
Percent 500:		Percent 1000:	
Melting Point (Measured):		Melting Point (est):	MPD NaN °C (Exp.) (EPI): 282.0794982910156 °C (Est., Joback) 119.01715087890625 °C (Est., Gold) 151.62960815429688 °C (Est., Selected) 1.9112759042637781%
Vapor Pressure:		Vapor Pressure (est): 0.000012	VP (EPI): NaN mmHg (Exp.) 8.776204236904395E-8 Pa (Est., Antoine) 6.582712708258498E-10 mmHg (Est., Antoine) 5.925547576351211E-7 Pa (Est., Grain) 4.444538468033191E-9 mmHg (Est., Grain) 1.3811481717325024E-4 Pa (Est., Mackay) 1.0359491844800576E-6 mmHg (Est., Mackay) 5.925547576351211E-7 Pa (Est., Selected) 4.444538468033191E-9 mmHg (Est., Selected) 1.155788608437547E-5 Pa (Est., SubCooled) 8.669151441154099E-8 mmHg (Est., SubCooled)
Water Solubility:		Water Solubility (EST): 1000	Water Solubility (Exp.): NaN (EPI): 3518.090087890625 (Est.)

Log Kow:	Log P	Log NaN (Exp.) 1.21
Log P:	Comment:	Kow (EPI): (Est.)

SAT Concern

Ecotox Rating (1):	Ecotox Rating (1):	Comment (1):
Ecotox Rating (2):	Ecotox Rating (2):	Comment (2):
Health Rating (1):	Health Rating (1):	Comment (1):
Health Rating (2):	Health Rating (2):	Comment (2):

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
3	1	2 (ECO)	

Exposure Based Review (Health)?	N
Exposure Based Review (Ecotox)?	N
SAT IRR-E, SENS; CORR;	
Keywords: AquaTox	

Fate Assessment P-18-0152

Summary: FATE: Estimations for the low weight, monomer species, MW = [REDACTED] with MP < 25 °C (E)

$\log K_{ow} = -1.41$ (E)
 $S > 10$ g/L at 25 °C (E)
 $VP = 1.2E-4$
 torr at 25 °C (E)
 $BP = 292$ °C (E)
 $H < 1.00E-8$ (E)
 $\log K_{oc} =$
 2.60 (E)
 $\log \text{Fish BCF} = 0.50$ (3) (E)
 $\log \text{Fish BAF} = -0.05$ (1) (E)

POTW removal (%) = 0-25 via sorption; Analog [REDACTED]: OECD 301B(Mod Sturm CO2 ev): 3.22-6.89%/29 d. NRB.
 Time for complete ultimate aerobic biodeg > mo
 Sorption to soils/sediments = moderate
 PBT Potential: P3B1
 *CEB FATE: Migration to ground water = moderate
 Bioconcentration factor to be put into E-FAST: 1

PMN

Material:

Overall wastewater treatment removal is 0-25% via sorption.

Sorption to sludge is low based on estimated physical-chemical properties from EPISUITE.

Air Stripping (Volatilization to air) is negligible based on estimated physical-chemical properties from EPISUITE.

Removal by biodegradation in wastewater treatment is negligible based on the measured data for an analog [REDACTED] OECD 301B(Mod Sturm CO2 ev): 3.22-6.89%/29d NRB).

The aerobic aquatic biodegradation

half-life is greater than months based on the measured data for an analog [REDACTED] OECD 301B(Mod Sturm CO2 ev): 3.22-6.89%/29d NRB).

The

anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.

Sorption to soil and sediment is moderate based on estimated physical-chemical properties from EPISUITE.

Migration to groundwater is moderate based on estimated physical-chemical properties from EPISUITE.

PMN Material:

High

Persistence (P3) is based on the aerobic and anaerobic biodegradation half-lives.

Low Bioaccumulation potential (B1) is based on BCFBAF model estimates.

Bioconcentration/Bioaccumulation factor to be put into E-Fast: 1.

Removal in 0-25

WWT/POTW

(Overall):

Condition	Rating Values w/ Rating Description	Comment
WWT/POTW	1	
Sorption:		
WWT/POTW	4	
Stripping:		
Biodegradation	4	
Removal:		
Biodegradation		
Destruction:		
Aerobic Biodeg	4	
Ult:		
Aerobic Biodeg		
Prim:		
Anaerobic Biodeg	4	
Ult:		
Anaerobic Biodeg		
Prim:		
Hydrolysis (t1/2		
at pH 7,25C) A:		
Hydrolysis (t1/2		
at pH 7,25C) B:		
Sorption to	3	
Soils/Sediments:		
Migration to	3	
Ground Water:		
Photolysis A,		
Direct:		

Condition	Rating Values w/ Rating Description	Comment
Photolysis B, Indirect: Atmospheric Ox A, OH: Atmospheric Ox B, O3:		

Health Assessment

Health Summary: The absorption is expected to be poor dermally, good by the lungs and poor in the GI tract based on p-chem properties. There is concern for corrosion due to the pH [REDACTED] (SDS), eye irritation and sensitization based on an analog.

Routes of Dermal , Oral,
Exposure: Inhalation

Test Data Submitted

Test Data Analog
Submitted: [REDACTED] In Vivo Dermal Irritation
 Negative,
 In Vivo Eye Irritation Positive, Guinea Pig Dermal Sensitization Positive,
 Oral LD50 = 196 mg/kg, Dermal LD50 > 2000 mg/kg, LC50 > 0.6 mg/L,
 Ames Test Negative with and without metabolic
 activation

Ecotox Assessment

Test organism	Test Type	Test Endpoint	Predicted	Measured	Comments
Fish	96-h	LC50	3.7		Predictions are based on hazard data from an analogous chemical [REDACTED]
Daphnid	48-h	LC50	34		Predictions are based on hazard data from an analogous chemical [REDACTED]
Green Algae	96-h	EC50	0.036		Predictions are based on hazard data from an analogous chemical [REDACTED]
Fish	-	Chronic Value	0.37		Predictions are based on hazard data from an analogous chemical [REDACTED] with an ACR of 10
Daphnid	-	Chronic Value	3.4		Predictions are based on hazard data from an analogous chemical [REDACTED] with an ACR of 10
Green Algae	-	Chronic Value	0.032		Predictions are based on hazard data from an analogous chemical [REDACTED]

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic:	36	4	9	The acute COC is based on the algal EC50 from an analogous chemical [REDACTED].
Chronic Aquatic:	32	10	3	The chronic COC is based on the algal ChV from an analogous chemical [REDACTED]

Ecotox Route of Exposure? All releases to water

Factors	Values	Comments
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Factors	Values	Comments
SARs:		Not applicable since the environmental assessment was conducted using analogue test data
SAR Class:		Not applicable since the environmental assessment was conducted using analogue test data
TSCA NCC Category?	Aliphatic Amines	

Recommended Testing

Ecotox

Value Comments

EPA estimated environmental hazard of this new chemical substance using hazard data on an analogous chemical [REDACTED]; MW [REDACTED]; Log Kow = -1.41 (P, Monomer), -0.26 (P, Dimer), 0.19 (P, Trimer), 0.64 (P, Tetramer), 1.09 (P, Pentamer); Liquid (est.) with an unknown MP (P); S = 1E+6 mg/L (P, Monomer), 740600 mg/L (P, Dimer), 126000 mg/L (P, Trimer), 73100 mg/L (P, Tetramer), 10500 (P, Pentamer); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO₃; and TOC <2.0 mg/L.

Ecotoxicity Test Data Results for P-18-0152:

Fish Ecotoxicity Test:

Health and

Environmental Sciences of [REDACTED] conducted a 96-hour acute toxicity test in rainbow trout (*Oncorhynchus mykiss*) with an acceptable analog substance [REDACTED] under static conditions. The test item was assumed pure as received. This study followed OECD test guideline No. 203 (1992) and EU Method C.1 (1992). Following a range-finding study, two replicates of ten *O. mykiss* were exposed to a dilution water control (well water) or the test substance at a nominal concentration of 0.31, 0.63, 1.3, 2.5, 5.0, or 10 mg/L. Measured concentrations for the three highest test concentrations ranged from 109-152% of nominal values at test initiation and from 111-168% of nominal values at test termination, based on ICP-OES analysis. Because the LOQ for the ICP method was 2.5 mg/L on day 0 and 1.7 mg/L on day 0, test concentrations below 2.5 mg/L could not be analytically verified. A primary stock solution was prepared by dissolving the test article in well water at a concentration of 500 mg/L. The primary stock was inverted at least 20 times to mix the test article. The primary stock solution appeared clear and colorless. The test solutions

were prepared by proportional dilution of the primary stock with well water. After addition of the appropriate amount of primary stock, each test solution was mixed with a glass stir rod. All test solutions appeared clear and colorless. Over the course of the study, temperature ranged from 11.8-12.1°C, pH ranged from 8.0-8.4 and dissolved oxygen ranged from 8.3-9.8 mg/L. Dilution water hardness ranged from 70-82 mg/L as CaCO₃. A loading rate of 0.19 g/L was reported. The percent mortality at 0 (control), 0.31, 0.63, 1.3, 2.5, 5.0, and 10 mg/L was 5%, 5%, 0%, 10%, 20%, 80%, and 75%, respectively. No sub-lethal effects were observed during the study. Based on analytically verified nominal test concentrations, the 96-hour LC₅₀ was 3.7 mg/L. This is an acceptable test.

96-hour LC₅₀ = 3.7 mg/L

Daphnid Ecotoxicity Test:

Health and

Environmental Sciences of [REDACTED] conducted a 48-hour acute toxicity test on in the water flea (*Daphnia magna*) with an acceptable analog substance [REDACTED] under static conditions. The test item was assumed pure as received. This study followed OECD test guideline No. 202 (1984) and EU Method C.2 (1992). Two replicates of ten *D. magna* were exposed to a dilution water control (well water) or the test substance at a nominal concentration of 10, 18, 32, 56, or 100 mg/L. Measured concentrations ranged from 90-102% of nominal values at test initiation and from 89-96% of nominal values at 48 hours, based on ICP-OES analysis (LOQ = 1.4 mg/L at 0 hours and 1.65 mg/L at 48 hours). The test solutions were prepared by direct addition of the test article to each test solution. Test article was weighed into tared glass weighing caps which were added to one-liter volumetric flask partially filled with well water. Actual test article weights used to generate nominal concentrations were 0, 0.010, 0.018, 0.032, 0.056, and 0.100 g. All solutions were mixed by repeated inversions until test article dispersed and brought to appropriate volume with well water. Test solutions were then distributed into duplicate labeled 250 mL glass beakers, which served as the test vessels. Each test vessel was covered with a watch glass to reduce evaporation. Over the course of the study, temperature ranged from 20.2-20.9°C, pH ranged from 8.09-8.64 and dissolved oxygen ranged from 8.52-8.96 mg/L. Dilution water hardness ranged from 92-124 mg/L as CaCO₃. A loading rate of 50 g/L was calculated. The percent mortality at 0 (control), 10, 18, 32, 56, and 100 mg/L was 0%, 5%, 0%, 45%, 95%, and 100%, respectively. The single mortality at 10 mg/L was not considered dose-related and was therefore not included in analysis. Based on nominal test concentrations, the 48-hour EC₅₀ was 34 mg/L. This is an acceptable test.

48-hour EC₅₀ = 34 mg/L

Algal Ecotoxicity Test:

Health and

Environmental Sciences of [REDACTED] conducted a 96-hour growth

inhibition test in green algae (*Selenastrum capricornutum* Printz) with an acceptable analog substance [REDACTED] under static conditions. The test item was assumed pure as received. This study followed OECD test guideline No. 201 (1984). Following a range-finding study, four replicates of *S. capricornutum* (approx. 1×10^4 cells/mL) were exposed to the test substance at nominal concentrations of 3, 10, 18, 56, or 100 µg/L. Additionally, 4 control replicates of *S. capricornutum* were exposed to algal medium only. Analytical confirmation of concentration and stability was not performed. The algal cultures were illuminated with a light intensity of 4300 ± 1075 . A stock solution of 10,000 µg/L was prepared by addition of 0.010 grams test article into a sterile glass cap. The cap was subsequently added into a sterile 1 L volumetric flask containing sterile AAM test medium. After the test article was added, the stock solution was mixed vigorously by hand and brought up to volume with additional sterile AAM test medium. The stock solution was diluted to prepare the nominal test concentrations. Over the course of the study, temperature ranged from 23.5-24.1°C and pH ranged from 7.28-7.97. The mean cell density of control cultures increased by a factor of 190 within 96 hours. Based on nominal concentrations, the 96-hour EC50 values were 0.076 mg/L for growth rate and 0.036 mg/L for biomass. The 96-hour NOEC and LOEC values, respectively, were 0.056 and 100 mg/L for growth rate, and 0.018 and 0.056 mg/L for biomass. The corresponding 96-hour ChV values were calculated to be 0.075 mg/L for growth rate, and 0.032 mg/L for biomass. This is an acceptable test.

Growth Rate:

96-hour EC50 = 0.076 mg/L

96-hour NOEC = 0.056 mg/L

96-hour LOEC = 0.100 mg/L

96-hour ChV = 0.075
mg/L

Biomass:

96-hour EC50 = 0.036 mg/L

96-hour NOEC = 0.018 mg/L

96-hour LOEC = 0.056 mg/L

96-hour ChV = 0.032 mg/L

Daphnid

Ecotoxicity Test:

[REDACTED] Toxicology Department conducted a 21-day chronic toxicity test in the water flea (*Daphnia magna*) with an acceptable analog substance (CASRN: [REDACTED]; purity not provided) under static conditions. No study guideline was specified. The study was run in triplicate where two replicates of five *D. magna* were exposed to a dilution water control (reconstituted water) or the test substance at a nominal concentration of 0.01,

0.03, 0.1, 0.3, 1.0 mg/L. The chemical was added to 600 mL beakers, each containing 400 mL of hard reconstituted water. Analytical confirmation of concentration and stability was not performed. Temperature, pH, and dissolved oxygen measurements for the test solutions were not reported. A loading rate of 12.5 daphnid/L was calculated. No mortalities occurred at concentrations \leq 0.3 mg/L; scattered mortalities occurred in the controls (1.7-3.3%) and highest test concentration (8.1-10%). No effect was observed on reproductive success up to 0.30 mg/L. A slight decrease in young produced was observed at 1 mg/L; however, this decrease was not statistically significant. Survival of the F1 generation – measured only for the first 24 hours – was high for all test concentrations and the control. Based on nominal test concentrations, the 21-day NOEC was 1 mg/L. There are deficiencies with this study (a static chronic study; no purity; no p/chem. properties; no analytical confirmation; etc.). As a result, this is not an acceptable study.

21-day NOEC = 1 mg/L

Conclusions

██████████ (sponsor) submitted three acceptable ecotoxicity studies (fish, aquatic invertebrate and algae) on an acceptable analog substance ██████████ for P-18-0152 (see above). Due to multiple deficiencies (see above) in the chronic *Daphnia magna* study (a fourth study), it is not considered acceptable. Based on a read-across approach from an acceptable analog ██████████ to P-18-0152, the “acute” fish, aquatic invertebrate, and algal endpoint values are 3.7, 34, and 0.036 mg/L, respectively. Based on a read-across approach from an acceptable analog ██████████ to P-18-0152, the “chronic” fish, aquatic invertebrate, and algal endpoint values (chronic values; ChVs) are 0.37, 3.4, and 0.032 mg/L, respectively. Acute to chronic ratios (ACRs) of 10 were used to derive the fish and aquatic invertebrate ChVs) for P-18-0152.

The acute concentration of concern (COC) for P-18-0152, based on read-across algal data from ██████████, is 0.009 mg/L (algae 96-hr EC50 value of 0.036 mg/L / assessment factor of 4). The chronic COC for P-18-0152, based on the algal chronic value (0.032 mg/L), is 0.003 mg/L (algal chronic value divided by an assessment/uncertainty factor of 10).

Acute COC = 9 ppb
Chronic COC = 3 ppb

Ecotox Reviewer:
J. Gallagher
Date: 5/3/2018

Ecotox Factors Comments

Environmental

Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using hazard data on an analogous chemical [REDACTED]

Based on analogue test data [REDACTED] the acute toxicity values estimated for fish, aquatic invertebrates, and algae are 3.7 mg/L, 34 mg/L, and 0.036 mg/L, respectively. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are 0.37 mg/L (analogue test data with an ACR of 10), 3.4 mg/L (analogue test data with an ACR of 10), and 0.032 mg/L (analogue test data), respectively. These toxicity values indicate that the new chemical substance is expected to have high environmental hazard. Application of assessment factors of 4 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern of 0.009 mg/L (9 ppb) and 0.003 mg/L (3 ppb), respectively.

Environmental Risk: Risks to the environment were evaluated by comparing estimated surface water concentrations with the acute and chronic concentrations of concern. Risks to the environment were not identified due to releases to water that did not exceed the acute COC or chronic COC.